

Carbamic acid, ethyl-, methyl ester
6135-31-5 | DTXSID80210261

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.31 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.68e-01

Confidence level: 5.96e-01

Nearest Neighbors from the Training Set

Image not found

N-Methylacetamide

Measured: 13.7

Predicted: 6.03

Image not found

Methyl nicotinate

Measured: 3.47e-01

Predicted: 4.31e-01

Image not found

Hydrazinecarboxamide, 2-(1-methylethylidene)-

Measured: 5.40e-01

Predicted: 4.98e-01

Image not found

Propyl carbamate

Measured: 7.41e-01

Predicted: 1.25

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1-cyanoethyl acetate

Measured: 1.77

Predicted: 1.78